Boson-fermion demixing in a cloud of lithium atoms in a pancake trap

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Abstract.   We evaluate the equilibrium state of a mixture of ^{7}Li and ^{6}Li atoms with repulsive interactions, confined inside a pancake-shaped trap under conditions such that the thickness of the bosonic and fermionic clouds is approaching the values of the s-wave scattering lengths. In this regime the effective couplings depend on the axial confinement and full demixing can become observable by merely squeezing the trap, without enhancing the scattering lengths through recourse to a Feshbach resonance.

PACS numbers: 03.75.-b, 05.30.-d, 73.43.Nq

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1. Introduction

Dilute boson-fermion mixtures have recently been studied in several experiments by trapping and cooling gases of mixed alkali-atom isotopes [1, 2, 3, 4, 5, 6]. The boson-fermion coupling strongly affects the equilibrium properties of the mixture and can lead to quantum phase transitions. In particular, it has been shown that boson-fermion repulsions in three-dimensional (3D) clouds can induce spatial demixing of the two components when the interaction energy overcomes the kinetic and confinement energies [7]. Several configurations with different topology are possible for a demixed cloud inside a harmonic trap [8]. Although spatial demixing has not yet been experimentally observed, the experiments of Schreck *et al.* [1] on a ^{6}Li-^{7}Li mixtures inside an elongated 3D trap appear to be not far from the onset of a demixed state: an increase in the boson-fermion scattering length by a factor five would be needed to enter the phase-separated regime [9].

In this Letter we examine the possibility of attaining phase separation by merely varying the trap geometry for the ^{6}Li-^{7}Li mixture at the "natural" values of the scattering lengths. We focus on the case of quasi-two-dimensional (Q2D) confinement inside a pancake-shaped trap. We find that this geometry favours the demixed state through the appearance of the axial size of the atomic clouds in their effective coupling in the azimuthal plane. We also show that several configurations are possible in the plane of the trap at zero temperature, but the configuration consisting of a core of bosons surrounded by a ring of fermions is the most energetically favourable for a wide range of values of system parameters.

2. The model

The atomic clouds are trapped in pancake-shaped potentials given by

$$V_{b,f}^{ext}(x,y,z) = m_{b,f}\omega_{x(b,f)}^2(x^2 + \lambda_{b,f}^2 y^2)/2 + m_{b,f}\omega_{z(b,f)}^2 z^2/2 \equiv V_{b,f}(x,y) + U_{b,f}(z) \quad (1)$$

where $m_{b,f}$ are the atomic masses and $\omega_{z(b,f)} \gg \omega_{x(b,f)}$ the trap frequencies. We focus on the case where the trap is flat enough that the dimensions of the clouds in the axial direction, which are of the order of the axial harmonic-oscillator lengths $a_{z(b,f)} = (\hbar/m_{b,f}\omega_{z(b,f)})^{1/2}$, are comparable to the 3D boson-boson and boson-fermion scattering lengths a_{bb} and a_{bf}. In this regime we can study the equilibrium properties of the mixture at essentially zero temperature ($T \simeq 0.02\,T_F$) in terms of the particle density profiles in the $\{x,y\}$ plane, which are $n_c(x,y)$ for the Bose-Einstein condensate and $n_f(x,y)$ for the fermions. The profiles are evaluated using the Thomas-Fermi approximation for the condensate and the Hartree-Fock approximation for the fermions. We shall take $a_{zb} = a_{zf}$ ($= a_z$, say) and only near the end we shall discuss the case $\lambda_{b,f} \neq 1$.

The Thomas-Fermi approximation assumes that the number of condensed bosons is large enough that the kinetic energy term in the Gross-Pitaevskii equation may be

neglected [10]. It yields

$$n_c(x, y) = [\mu_b - V_b(x, y) - g_{bf} n_f(x, y)]/g_{bb} \tag{2}$$

for positive values of the function in the square brackets and zero otherwise. Here, μ_b is the chemical potential of the bosons. This mean-field model is valid when the high-diluteness condition $n_c a_{bb}^2 \ll 1$ holds and the temperature is outside the critical region. If the conditions $a_z > a_{bb}, a_{bf}$ are fulfilled, the atoms experience collisions in three dimensions and the coupling constants in Eq. (2) can be written in terms of the 3D ones as [11]

$$g_{bb} = \frac{g_{bb}^{3D}}{\sqrt{2\pi}a_z}, \quad g_{bf} = \frac{g_{bf}^{3D}}{\sqrt{2\pi}a_z} \tag{3}$$

with $g_{bb}^{3D} = 4\pi\hbar^2 a_{bb}/m_b$, $g_{bf}^{3D} = 2\pi\hbar^2 a_{bf}/m_r$ and $m_r = m_b m_f/(m_b + m_f)$.

The Hartree-Fock approximation [12, 13, 14] treats the fermion cloud as an ideal gas subject to an effective external potential, that is

$$n_f(x, y) = \int \frac{d^2p}{(2\pi\hbar)^2} \left\{ \exp\left[\left(\frac{p^2}{2m_f} + V^{eff}(x, y) - \mu_f \right) / k_B T \right] + 1 \right\}^{-1}, \tag{4}$$

where μ_f is the chemical potential of the fermions and

$$V^{eff}(x, y) = V_f(x, y) + g_{bf} n_c(x, y). \tag{5}$$

The fermionic component has been taken as a dilute spin-polarized gas, for which the fermion-fermion *s*-wave scattering processes are inhibited by the Pauli principle and *p*-wave scattering is negligibly small [15]. In the mixed regime the Fermi wave number in the azimuthal plane should be smaller than $1/a_{bf}$, but this is not a constraint in the regime of demixing where the boson-fermion overlap is rapidly dropping.

The chemical potentials $\mu_{b,f}$ characterize the system in the grand-canonical ensemble and are determined by requiring that the integrals of the densities over the $\{x, y\}$ plane should be equal to the average numbers N_b and N_f of particles. The presence of a bosonic thermal cloud can be treated by a similar Hartree-Fock approximation [9], but it has quite negligible effects at the temperatures of present interest.

3. General conditions for phase separation

The effective strength of the atom-atom collisions in the azimuthal plane depends in our Q2D model on the axial harmonic-oscillator length according to Eq. (3). We derive and illustrate in this section the consequences for demixing at very low temperatures.

We preliminarily recall that in the macroscopic limit the phase transition is sharp and the overlap between the two species after demixing is restricted to the interfacial region, where it is governed by the surface kinetic energy (see Ref. [16] for an example in a 3D model). In the case of mesoscopic clouds under confinement the transition is instead spread out and several alternative definitions of the location of demixing can

therefore be given. We discuss below three alternative locations, that we denote as partial, dynamical, and full demixing. Their definition and the derivation of simple analytical expressions in the Q2D model are given in the following.

3.1. Partial demixing

The interaction energy E_{int} between the boson and fermion clouds initially grows as the boson-fermion coupling is increased, but reaches a maximum and then falls off as the overlap between the two clouds diminishes. We locate partial demixing at the maximum of E_{int}, that we calculate from the density profiles according to the expression

$$E_{int} = g_{bf} \int dx\, dy\, n_c(x,y)n_f(x,y). \tag{6}$$

In the calculations that we report in this section we have used values of system parameters as appropriate to the experiments in Paris on the ^{6}Li-^{7}Li mixture [1], that is $N_b = N_f \simeq 10^4$ and $\omega_{xb}/2\pi = 4000$ Hz, $\omega_{xf}/2\pi = 3520$ Hz.

We first fix the two scattering lengths at their "natural" values ($a_{bb} = 5.1\,a_0$ and $a_{bf} = 38\,a_0$, with a_0 the Bohr radius) and vary the thickness a_z of the trap from $100\,a_{bf}$ down to a_{bf}. By this choice we are increasing both the boson-boson and the boson-fermion effective coupling in the azimuthal plane. The behaviour of the interaction energy as a function of the ratio a_{bf}/a_z at fixed a_{bb} and a_{bf} is shown in Fig. 1. It is seen that E_{int} goes through a maximum at $a_z \simeq 16\,a_{bf}$.
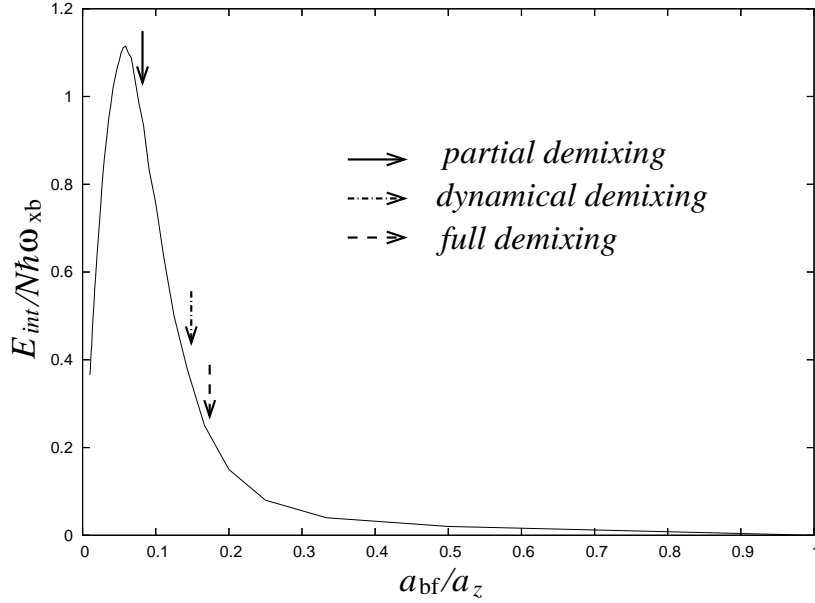
Figure 1. Boson-fermion interaction energy E_{int} in a circular disc (in units of $N\hbar\omega_{xb}$, with $N = N_b + N_f$), as a function of a_{bf}/a_z for fixed values of a_{bb} and a_{bf}. The arrows indicate the locations of demixing estimate from Eqs. (7), (12) and (14).

As an alternative and with the aim of a later comparison with the results previously obtained in the 3D case [8, 9], we show in Fig. 2 the interaction energy as a function of the ratio a_{bf}/a_{bb} at fixed a_{bb}. The axial thickness a_z has been set equal to the largest of the two scattering lengths. This condition fixes the limit of validity of our model [17]. The maximum of E_{int} lies at $a_{bf}/a_{bb} \simeq 0.8$, much below the value $a_{bf}/a_{bb} \simeq 7$ of the ratio of the "natural" scattering lengths. In fact, at $a_{bf}/a_{bb} \simeq 7$ the two clouds would undergo demixing as the axial trap stifness is increased towards a Q2D model.
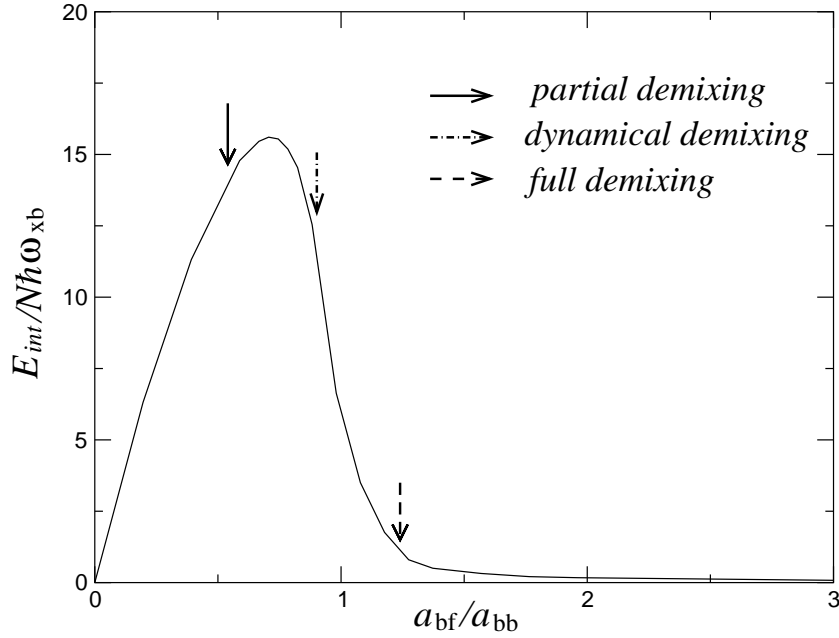
Figure 2. Boson-fermion interaction energy E_{int} in a circular disc (in units of $N\hbar\omega_{xb}$), as a function of a_{bf}/a_{bb} for $a_{bb} = 5.1\,a_0$. The arrows indicate the locations of demixing estimate from Eqs. (7), (12) and (14).

An approximate analytic formula for the location of partial demixing as a function of the system parameters in the Q2D model can be obtained from the condition $\partial E_{int}/\partial g_{bf} = 0$ by using the estimate $n_{c,f} \approx N_{b,f}/(2\pi R_{b,f}^2)$ with the values of the cloud radii in the absence of boson-fermion interactions, $R_f = (8N_f/\lambda_f)^{1/4} a_{xf}$ and $R_b = (16N_b a_{bb}/(\sqrt{2\pi}a_z\lambda_b))^{1/4} a_{xb}$ where $a_{x(b,f)} = (\hbar/m_{b,f}\omega_{x(b,f)})^{1/2}$. The location of the maximum in the boson-fermion interaction energy as a function of a_{bf}/a_{bb} lies at

$$\left.\frac{a_{bf}}{a_{bb}}\right|_{part} \simeq \gamma_{part} \left(\frac{a_z}{a_{bb}}\right)^{1/2} \tag{7}$$

where

$$\gamma_{part} = \left(c_1 \frac{N_f^{1/2}}{N_b^{1/2}} + c_2 \frac{N_b^{1/2}}{N_f^{1/2}}\right)^{-1} \tag{8}$$

with

$$c_1 = \left(\frac{2}{\pi}\right)^{1/4} \frac{m_f \omega_{xf}}{2m_r \omega_{xb}} \left(\frac{\lambda_f}{\lambda_b}\right)^{1/2} \tag{9}$$

and

$$c_2 = \left(\frac{2}{\pi}\right)^{1/4} \frac{m_b \omega_{xb}}{2m_r \omega_{xf}} \left(\frac{\lambda_b}{\lambda_f}\right)^{1/2}. \tag{10}$$

We recognise in Eq. (8) a geometric combination of two scaling parameters: $c_1 N_f^{1/2}/N_b^{1/2}$ is dominant in the case $N_b \ll N_f$ while $c_2 N_b^{1/2}/N_f^{1/2}$ is dominant in the opposit limit. The prediction obtained from Eq. (7) is shown in Figs. 1 and 2 by a solid arrow. There clearly is good agreement between the analytical estimate and the numerical results.

3.2. Dynamical demixing

On further increasing the boson-fermion coupling one reaches the point where the fermion density vanishes at the centre of the trap. This occurs when

$$\left.\frac{g_{bf}}{g_{bb}}\right|_{dyn} = \frac{\mu_f}{\mu_b}. \tag{11}$$

We denote this point as the dynamical location of the demixing in a mesoscopic cloud, since we expect a sharp upturn of the low-lying fermion-like collective mode frequencies to occur here as it is the case for both collisional and collisionless excitations in a mixture under 3D confinement [18, 19].

If we insert the chemical potentials for ideal-gas clouds in Eq. (11), we obtain an approximate expression for the location of dynamical demixing,

$$\left.\frac{a_{bf}}{a_{bb}}\right|_{dyn} \simeq \gamma_{dyn}\left(\frac{a_z}{a_{bb}}\right)^{1/2} \tag{12}$$

where

$$\gamma_{dyn} = \left(\frac{\pi}{2}\right)^{1/4}\frac{2m_f}{m_b+m_f}\frac{\omega_{xf}}{\omega_{xb}}\left(\frac{N_f\lambda_f}{N_b\lambda_b}\right)^{1/2}. \tag{13}$$

The condition for dynamical demixing coincides with that for partial demixing in the limit $N_b \gg N_f$. The prediction obtained from Eq. (12) is indicated in Figs. 1 and 2 by a dot-dashed arrow.

3.3. Full demixing

The point of full demixing is reached when the boson-fermion overlap becomes negligible as in a macroscopic cloud. Using the instability criterion outlined in Ref. [20] for the 3D case, the condition for full phase separation at $T = 0$ is

$$\left.\frac{a_{bf}}{a_{bb}}\right|_{full} \simeq \gamma_{full}\left(\frac{a_z}{a_{bb}}\right)^{1/2} \tag{14}$$

where

$$\gamma_{full} = \left(\sqrt{2\pi}\frac{2m_r}{m_b+m_f}\right)^{1/2}. \tag{15}$$

At variance for the condition for full phase separation in 3D, for the Q2D confinement this criterion does not depend on the number of fermions, while $1/a_z$ plays the role of the Fermi momentum.

The prediction obtained from Eq. (7) is indicated in Figs. 1 and 2 by a short-dashed arrow.

3.4. Density profiles at full demixing

In summary, it can be seen from Eqs. (7), (12) and (14) that the two control parameters for the transition in a mesoscopic cloud under Q2D confinement are a_{bf}/a_{bb} and a_z/a_{bb}. Our main conclusion is that in a Q2D geometry a relatively small value of the boson-fermion scattering length suffices to reach the regime of full phase separation. In the case of the ^{6}Li-^{7}Li mixture the bare values of the boson-boson and boson-fermion scattering lengths fulfill the condition for full phase separation for values of a_z lower than 10 a_{bf}.

In view of the above result, it is useful to illustrate in Fig. 3 the density profiles to be expected in the fully demixed regime for a mixture under isotropic confinement in the azimuthal plane (notice that a circular disc appears in Fig. 3 as an oval, because of the different scales used on the horizontal and vertical axes). In fact we have found various metastable configurations for the demixed mesoscopic cloud in addition to the thermodynamically stable one consisting of a core of bosons surrounded by a ring of fermions.

In Fig. 3 we show topviews of the density profiles in the $\{x, y\}$ plane for the choice of parameters $a_{bb} = 5.1\,a_0$, $a_{bf} = 38\,a_0$ and $a_z = a_{bf}$. The most energetically stable configuration is shown in Fig. 3(a) and lies at energy $E = 74.90\,N\hbar\omega_{xb}$. Figure 3(b) shows a configuration with fermions at the centre surrounded by a ring of bosons inside a fermion cloud ($E = 78.94\,N\hbar\omega_{xb}$). In Fig. 3(c) a fermion slice lies between two boson slices surrounded by a fermion cloud ($E = 79.04\,N\hbar\omega_{xb}$). Finally, Fig. 3(d) shows an asymmetric configuration in which a core of bosons is displaced away from the centre of the trap ($E = 80.20\,N\hbar\omega_{xb}$). The latter two configurations break the symmetry of the trap and this is an effect due to the finite size of the system.

Configurations (b)-(d) are structurally but not energetically stable, *i.e.* they represent metastable structures in local energy minima. They have been obtained by using density profiles with various topologies as the initial guess for the self-consistent solution of Eqs. (2) and (4). In experiments bulk modes with the appropriate symmetry may be exploited to attain these "exotic" configurations [21].

We have also studied the behaviour of the configurations shown in Fig. 3 as a function of the scattering lengths ($5.1a_0 < a_{bb} < 3 \times 10^5 a_0$ and $38a_0 < a_{bf} < 5 \times 10^7 a_0$) and the planar-anisotropy parameters ($10^{-3} < \lambda_{b,f} < 400$). In contrast to the case of an elongated 3D confinement studied in our previous work [8], where the lowest-energy configuration can have different topologies depending on the system parameters, we have found that the configuration shown in Fig. 3(a) remains the most energetically stable for the Q2D geometry. A configuration consisting of a central core of fermions surrounded by a cloud of bosons may, however, be the stable one for sufficiently strong boson-boson repulsions [8].
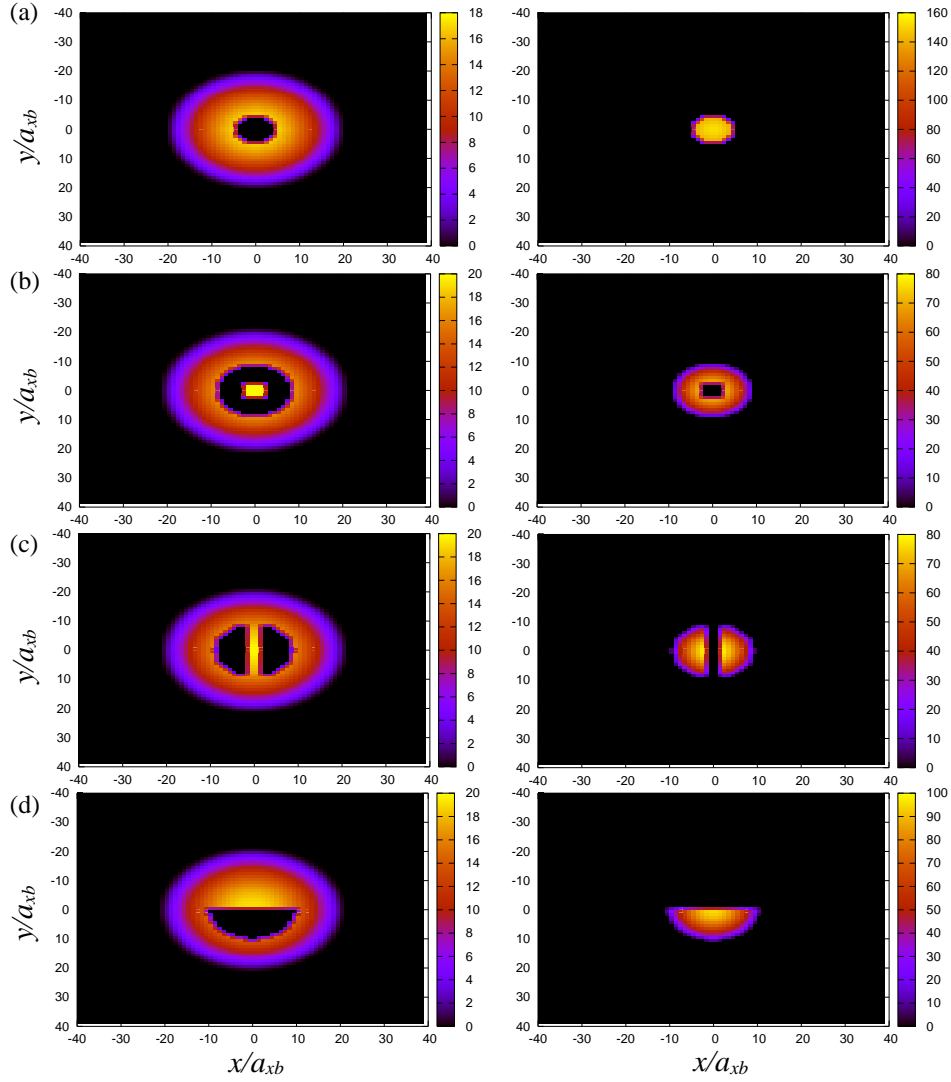
Figure 3. Density profiles at full demixing for fermions (left) and bosons (right) in the $\{x, y\}$ plane, for a Q2D mixture with $a_{bb} = 5.1\,a_0$, $a_{bf} = 38\,a_0$, and $\lambda_b = \lambda_f = 1$: (a) core of bosons surrounded by a ring of fermions; (b) core of fermions surrounded by a ring of bosons inside a fermion cloud; (c) fermion slice between two boson slices surrounded by a fermion cloud; (d) core of bosons displaced away from the centre of the trap and surrounded by a fermion cloud. Notice the difference in horizontal and vertical scales.

4. Summary and concluding remarks

In summary, we have focussed on a boson-fermion mixture confined inside pancake-shaped traps, such that the scattering events can still be considered three-dimensional but nevertheless affected by the vertical confinement. By using a mean-field description for the equilibrium densities in the azimuthal plane, we have studied the boson-fermion interaction energy as a function of the thickness of the atomic clouds and of the boson-boson and boson-fermion scattering lengths. We have given approximate analytical expressions identifying three critical regimes in terms of the scaling parameters a_{bf}/a_{bb} and a_z/a_{bb}: (i) partial demixing where the boson-fermion interaction energy attains maximum value from a balance between increasing interactions and diminishing overlap; (ii) dynamical demixing where the fermionic density drops to zero at the centre of the trap and a sharp dynamical signature of demixing may be expected; and (iii) full demixing where the boson-fermion overlap is negligible as in the macroscopic limit. These different criteria for the location of the phase transition in a mesoscopic cloud yield quite close predictions in a pancake-shaped trap under strong axial confinement.

We have found several metastable configurations for the demixed cloud, having various topologies but lying at higher energy above the stable configuration which is composed by a core of condensed bosons surrounded by fermions. We have verified that this is the minimum-energy configuration over extensive ranges of values for the coupling constants, the anisotropy in the plane of the trap, and the thickness of the trap.

A main result of our work is that full demixing can be reached in the ^{6}Li-^{7}Li mixture by merely tuning the thickness of the trap, without necessarily tuning the scattering lengths. The full-demixing critical value of about $10\,a_{bf}$ for the thickness is not attainable in the actual experiments with the bare value of the ^{6}Li-^{7}Li scattering length, and a combination of squeezing of the pancake-shaped trap and exploiting Feshbach resonances should be used. On the contrary, the dynamical location of demixing may be observed by only varying the number of particles, without enhancing the scattering length. In fact for a mixture of 10^6 atoms of ^{7}Li and 10^4 atoms of ^{6}Li trapped in the radial confinement discussed in Sec. 3.1, it may be possible to observe a sharp upturn of the low-lying fermionic modes for a pancake thickness of the order of $\sim 600\,a_{bf} \simeq 1\,\mu$m.

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